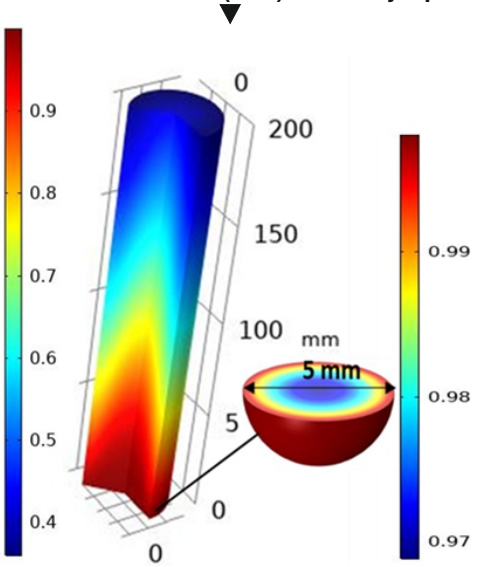
Double-Porosity Modeling

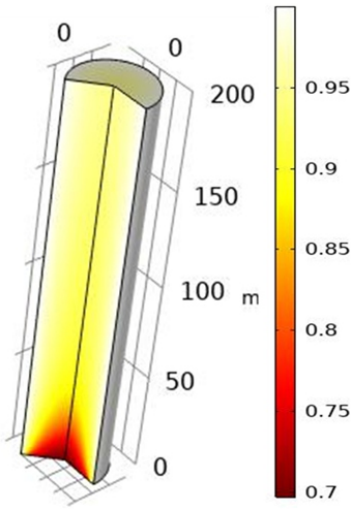
7

SO_3 Decomposition in Tubular-Packed Bed Reactor

Concentration profile (normalized) of SO_3 in Packed Bed Reactor (PBR) and catalyst particle



Temperature profile (normalized) in PBR



S. Sujeesh
Scientific Officer/E
Chemical Technology Division, Chemical Technology Group
Bhabha Atomic Research Centre (BARC), Trombay - 400 085, INDIA

A 'multi-scale' problem-heat and mass transport taking place in the macro-pores(voids) of the catalyst bed & heat, mass transport and reaction occuring in the micropores inside the catalyst particle-has been modeled for atalytic decomposition of SO_3, in a tubular-Packed Bed Reactor.

Hydrogen is considered as an excellent energy carrier, with potential to replace fossil fuels. Iodine-Sulphur (IS) and Hybrid-Sulphur (HyS) water splitting cycles are efficient and widely studied processes for mass production of H_2. Decomposition of sulphuric acid (H_2SO_4) is a three-step and energy intensive process in both, IS and HyS cycles.

A recent study (*Sujeesh et al., Sulphuric acid decomposition using Cr-Fe_2O_3 catalyst in a tubular Packed Bed Reactor (PBR): Modeling and experimental studies, Int. J. of Hydrogen Energy 2022, 47:11750-11763*), shows better experimental prediction with the developed double-porosity model, than isothermal-PBR and plug-flow (1-D) models for catalytic decomposition of SO_3 which is one of the three steps of decomposition of sulphuric acid. Also, multi-scale analysis of the reaction system using the double-porosity model, shows negligible film resistance as compared to pore diffusion resistance. Inside the pores concentration drop near the wall is found to be higher than that near the centre line, which is due to the faster intrinsic reaction kinetics near the high temperature wall than diffusion rate inside the pore.

Modeling of transport phenomena together with SO_3 decomposition reaction in two different porous-domains of a PBR is the novelty of the work. The developed model is useful to maximize the conversion of SO_3 in a PBR by minimizing the heat and mass transfer resistances.